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PARALLELIZATION OF ROCKET ENGINE SIMULATOR SOFTWARE

(P.R.E.S.S.)

INTERIM REPORT

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1. Background

Parallelization of Rocket Engine System Software (PRESS) project is part of a collaborative effort with Southern University at Baton Rouge (SUBR), University of West Florida (UWF), and Jackson State University (JSU).

The first-year funding, which supports two graduate students enrolled in our new Master's program in Computer Science at Hampton University and the principal investigator, have been obtained for the period form October 19, 1995 through October 18, 1996. The interim progress report, dated April 14, 1996, outlines the plans and progress in relevant sections:

Background
Hampton University's Research Infrastructure
Staffing for the Project
Project Task Assignments and Goals
Strategies Toward Achieving Stated Goals
Current Project Activities
Expected Challenges
Future Prospects and Conclusion

According to the overall task assignments detailed in the interim report, Hampton University's role is to collect the available software involving liquid-propellant rocket engines, place them in a common format and test to see they work, and finally, and most importantly, assure that fast execution is assured on parallel and supercomputer platforms.

Specifically, the work was experimentation with a large software package TDK (Two-Dimensional Kinetics) developed piecemeal over the period from 1986 to 1993 as part of RENS (Rocket Engine Numeric Simulator) project. To this end, we were able to check the correct performance of software on Sun4c and Cray Y-MP platforms. We have also made progress in the next step of translating Fortran source code, first to C language, and then to C++ in order to make further performance experimentation possible on the 64-node NCUBE parallel computer available on Hampton University's local area network.

The final report and request and plans for second year funding was filed on October 4, 1996. That report focused on the activities and accomplishments for the first year under the following topics:

Background -- The overall description of the three-year collaborative research
Research Progress Overview -- Work done from 10/1/95 to 10/1/96 on TDK package
Current Research Activities -- Mainly involving progress over Summer 1996)
Difficulties Encountered -- Concerning TDK's large size and inadequate documentation

Expected Challenges --	Concerning translation of Fortran code on mainframes to Borland C++ on PC platforms
Conclusion --	Redesign of TDK starting with high-level ad detailed requirements documents

Short of a coordinated effort involving various NASA centers and organizations within the Lewis Research Center and possibly other universities involved in the RENS collaborative research effort, the report outlined the plans for the second year funding for reworking of the current Fortran based TDK software. In a nutshell, the effort for the second year funding was characterized as: *major reworking, streamlining, redesign, and re-documentation of the TDK software, and the development of entirely new documentation.* Furthermore, the limitations of PC platform which was necessary for GUI interfaces were mentioned.

Through discussions and emails involving Mr. Ilesanmi Onawole who worked as the graduate research assistant only during the three months in Summer 1996, the principal investigator, and Messr. Ken Davidian and Don Noga of NASA Lewis Research Center, it was decided that it would be more productive to work on smaller and more manageable Fortran based rocket engine design software first and then tackle the larger size software packages like Two-Dimensional Kinetics (TDK). It was then decided that Hampton University, while still exploring alternatives for the reworking and re-documenting of TDK software, would obtain copies of the smaller size TURBDES, PUMPDES, and GASP software packages. To this end, a formal software use agreement was between Hampton University and NASA Lewis Research Center was prepared and approved by both parties. Thereafter, the second year funding stipend and tuition support for up to two graduate students was obtained. At the same time, a new graduate student, Ms. Chenhong Lu, was offered stipend support and joined the Hampton University's Master's Program in Computer Science. All focus shifted to the reworking and parallelization of TURBDES, PUMPDES, GASP, a cluster of loosely related software packages.

2. Research Progress Overview

In this section, we give an overview of progress since the final report of October 4, 1996. Upon notice for the second year funding, we have offered a 12-month stipend support with up to $ 4000.00 tuition allowance for a new applicant to our new Master's program, Ms. Chenhong Lu. Ms. Chenhong Lu, who is a Chinese national with F-1 student visa status, joined the graduate program in Fall of 1996. She has a Master's degree in Mathematics and excellent background in computer sciences. As promised with I-25, she was hired as the graduate student research assistant with 12-month stipend support. As she was going through the orientation in her graduate course enrollments and taking the work over from Mr. Ilesanmi, her mother became seriously ill, and she was allowed to withdraw for the duration of Fall semester 1996. Ms. Chenhong LU returned from China and resumed her graduate studies in Spring 1997. She was rehired as research assistant in this (PRESS) project for the period from January 1, 1997 through August 31, 1997.

The principal investigator during Fall 1996 and Spring 1996 semesters at 25% release time and Ms. Chenhong Lu during Spring 1997 have worked exclusively on the reworking of the above mentioned Fortran based software cluster. This effort is detailed in the next section.

3. Current Research Activities

The research since October 1996 has focused on downloading of the TURBDES/PUMPDES/GASP software cluster from Lewis Research Center and reconfiguration on HU's Cray Y-MP and SonOS NFS systems. While both the PI and the research assistant were getting familiar with the physical and mechanical design of liquid-propelled rocket engines through references [1,2], the above mentioned FORTRAN code was checked, compiled, debugged and successfully run on both platforms. Most of the effort, however, was expended on understanding the documentation for these packages and verification of the information contained therein. Although the documentation is far more clear and concise as opposed to TDK's, there were numerous discrepancies. These and various other challenges are discussed in the next section.

A significant activity was the attendance at R.E.N.S. Meeting and Review of Research Progress, University of West Florida, Pensacola, Florida, held during January 16-17, 1997. The meeting and research progress seminars and presentations involved all the participants of the overall RENS research effort. There, the PI presented the goals and plans for Parallelization of Rocket Engine System Software. Some of these are recapped below:

Hampton University's Charge

P.R.E.S.S. -- Parallelization of
Rocket
Engine
System
Software

- Involving for the First Year:

  TDK -- Two-Dimensional Kinetics

- for the Second Year:

  TURBDES -- Turbine Design (Point Perform.)
  PUMPDES -- Pump Design (Point Performance)
  GASP -- Gas Propellant (Point Performance)

PRESS Project Goals and Strategies (Second Year)

- Common platform for diverse software
  Porting and reconfiguration of RENS related software on HU computing facilities

- Accomplished for TDK software on Sun Workstations and Cray Y-MP (in FORTRAN)

- For TURBDES/PUMPDES software, glitches involving plotting subsystem require further testing and debugging work

- Improve performance and code efficiency through vectorization, optimization, and parallelization on HU's super/parallel computers

- **Strategy**:

  - Focus on TURBDES/PUMPDES with smaller scope (5 modules each as opposed to 282 for TDK software) and better documentation

  - Accomplish vectorizations, optimizations, and parallelization using CRAY Y-MP cf77 Fortran compiler with impressive benchmark results.

Tentative Goals and Strategy (Third Year)

- Demonstration and Promotion of Rocket Engine Software Suite

  - Interactive versions based on Borland C++ on PCs and AT&T C++ on SunOS workstations
  - GUI Improvements on BORLAND C++ version ObjectVision and JAVA extensions
  - Remote Access/Execution on Internet using JAVA applets and Demos on Wold Wide Web

- **Strategy**:

  - Focus on TURBDES/PUMPDES with smaller scope and clearer documentation

  - Translate into C first without worrying about object oriented design with classes, etc.

  - Graduate research assistants with proficiency in both FORTRAN and C/C++

Reworking and Parallelization of TURBDES/PUMPDES/GASP

Table 1 below gives the size of the TDK software which we previously worked on and found it to be unwieldy for the purpose of comparison. The details of work on TDK, including benchmark results, translations to C code, etc. have been discussed in the final report for the first year funding.

Table 1: 282-Module TDK Source Lines, Subroutines, and Commons.

Number of Lines	*File name*	*Description*
39388	tdk.src	Count of source lines all modules
2661	tod.com	Total number of COMMON declarations
263	tot.sub	Total number of subroutine declarations
260	tit.equ	Number of EQUIVALENCE declarations

Tables 2 gives the size of the PUMPDES and TURBDES packages. We do not provide any table for GASP since it is one large module.

Table 2: 8-Module TURBDES/PUMPDES Source Lines and Files

	Number of Lines	*File name*
PUMPDES		
	1034	pumpdes.for
	98	xbldlg.for
	342	xleak.for
	84	xnewton.for**
	186	xpmphd.for
	107	xtable.for
	1851	total
TURBDES		
	2459	gasp.f*
	2594	turbdes.for
	84	xnewton.for **
	107	xtable.for
	5244	total

* Module in a separate directory used by both PUMPDES and TURBDES
** Module Common to PUMPDES and TURBDES

4. Difficulties Encountered

The difficulties we encountered can best be categorized as a) Technical, b) Staffing, c) Equipment and software. Of these, except for the bureaucracy involving requisitioning process, the least important is the last one listed.

4.1 Technical

As is repeatedly reported by the graduate research assistant, the documentation, while far better than that of TDK, there are many inconsistencies. Furthermore, since the software was originally developed on DEC VAX/VMS platforms using non-standard VAX/VMS FORTRAN, there are problems with both the compilation process and the execution. One problem involved the calls to the SETUP module, which in turn, contained various plotting routines presumably related to DEC plotting and graphics. These are shown below:

```
Call from with SETUP.FOR Subroutine
-----------------------------------

C-----TOSS OUT TRAILING BLANKS ON AXIS TITLES
C-----DRAW AXIS TITLES
      CALL AXIS(XORG,YORG,AX,-NCX,XS,0.,XMINP,DX)
      CALL AXIS(XORG,YORG,AY,+NCY,YS,90.,YMINP,DY)
      CALL SYMBOL(XP,YP,0.14,TITLE,0.,NCT)
      CALL PLOT(1.5,1.5,-3)
      CALL PLOT(-1.0,-1.0,3)

      ..

      etc.
```

Since none of the plotting routines are available in the software which we downloaded, we had to exclude these calls in order to be able to proceed with compilation. Next there were numerous problems involving NAMELISTs which provide initialization and default parameters in external files (e.g., DFTTRB for default paramters, INTURB for initial paramters for TURBDES software, and similar ones for PUMDES software). Since those files were missing in the package, we reconstructed them using the available documentation.

At present, while we are able to produce executables, we are getting out-of-range outputs for many results. The main reason for this is the special internal representation of floating point real values in VAX hardware not agreeing with IEEE double precision standards. It appears that VAX representations provided slightly better precision for the real numbers.

4.2 Staffing

For staffing, we keep advertising through bulletin board notices, emails to the faculty, and discussions at departmental meetings. Partly due to the decreasing size of the graduate students enrolled in our graduate program, and partly to the interests of the graduate students on more popular areas (object-oriented software methodologies, java based software, ATM services in data communications, etc.), we have been unable hire a qualified graduate student from within our program. One other reason for this may be the challenging nature of the project in terms of its scope and definition. Finally, the reputation of the PI as highly "demanding" advisor does not help matters much.

Even if we could find willing graduate students, their knowledge is based on Pascal or Ada since these are the programming languages taught in our curricula. Interest in Fortran is more intense amongst non-majors (e.g., the PI teaches 40 non-majors in one class during Spring 1997 semester). However, these students totally lack any knowledge of UNIX, and in most cases, even MS-DOS. This closes out option of hiring a graduate student from other graduate programs at Hampton University, such as Mathematics, Physics, Chemistry, Electrical Engineering (although we hired Ilesanmi from the Electrical Engineering department with some success). On the other hand, the computer science majors are knowledgeably in Pascal and Ada, as mentioned before, and have interest only on C++ and Java. They have little or no interest in Fortran, for instance.

4.3 Equipment and Software

The delays and hindrances in the acquisitions of PC hardware from the budget which was provided only for the first year funding has been discussed in the first interim report dated April 12, 1996. For instance, due to the on-campus review and bidding process, we ended up with a 100-MHz CTX desktop instead of 200-MHz Pro200 from Micron requisitioned. However, the CTX desktop has sufficient disk space for the large Borland C++ Version 5.0 development suite (274 Megabytes). Since we have not yet translated any of the TURBDES/PUMPDES software into C++, we do not have a clear idea about execution speeds.

The main problem with equipment is excessive delays in requisitioning and the reluctance on the part of the university administration to do anything about it. There are also too stringent adherence to the various budget lines established, quite arbitrarily, by the university administration. Finally, there is a federal equipment audit scare where the researchers are told that the granting agencies are policing the equipment stringently. All in all, the problem which is probably prevalent in other institutions and not specific to this institution, is the university administration not being satisfied with the lavish percentages allocated to the administrative overhead items. It is therefore suggested that the granting institutions pay special attention to this and not cut out the principal investigators altogether from the research project budgeting.

5. New Directions for Second Year Funding

Primarily stemming from the discussions at the RENS Meeting in Pensacola, Florida in January of 1997, the new impetus for the RENS projects in general, and PRESS specifically, is closer cooperation with LeRC's Numerical Propulsion System Simulator (NPSS) organizations. NPSS operates several intra-net clusters of various kinds of computers and, in addition, under the acronym ARTT for Advanced Reusable Transportation Technology, develops simulators for aerodynamic and rocket systems combined. It was, therefore, suggested by Joe Hemminger at the meeting that the PI's working on RENS related grants establish closer contact with the technical staff of NPSS organization. Furthermore, a new kind of challenge was articulated whereby projects such as ours aim to access and execute diverse rocket engine system simulator software packages over LANs and intra-net clusters. As a starter, we discussed the p4 software tool to accomplish this over LANs. This tool, later enhanced under the new name of MPI (message passing interface and library), provides mechanism for executing code in parallel over LANs, in particular, over Sun Network File System based local area networks. The demo programs, however, are almost always in C rather than FORTRAN. This new direction appears to be more in line with NASA's overall objectives concerning rocket engine design software, and therefore, we wanted to direct PRESS project efforts toward these aims. These aims differ from the earlier goals articulated in these reports, such as code translations to an object-oriented base (C++ and ultimately Java) for better redesign or redesign options), GUI enhancements on PC platforms, and so forth. One other key issue in this regard is discussed next.

Another practical and potentially fruitful approach was suggested by Anthony Williams. This involved the C++ wrapper code around working Fortran based software modules (thus saving the translation effort). This idea appeared especially attractive to us since, even with the tool such as Argonne's MPI could easily incorporate C++ based message passing facilities. Further, after the C++ wrappers are successfully implemented, redesign along object-oriented principles becomes feasible.

In any case, up until the teleconference with Joe Hemminger, Rich Blech, and Angela Quealy, we have pursued this idea vigorously, first with Anthony Williams, and later with other NPSS staff, in order to obtain demonstrative software samples. For this purpose, and for the purpose of finding tools with wider scope than Argonne's MPI, we have set up a teleconfence on April 25, 1995. Indeed, this interim report awaited the result of that teleconference which, to us, was crucial.

At the teleconference which included the principal investigator, Messr. Joe Hemminger and Rich Blech, and Ms. Angela Clevely, we discussed various options and alternatives. It appeared that there were certain proprietary concerns involving C++ wrapper code samples. We have decided to obtain Argonne's tools PVM and MPI from their web site. We then would experiment with TURBDES/PUMPDES package both on Hampton University's hardware platforms but also on NPSS's LACE cluster (where the PI was granted an account). We further decided to keep in close contact and on the lookout for other tools that may be or become available.